**Amendment To The Claims**

The following amendments do not constitute an admission regarding the patentability of the amended subject matter and should not be so construed. Applicants reserve the right to pursue the subject matter of the canceled claims in this or any other appropriate patent application.

**Listing of Claims:**

1. (Previously presented) A method for generating coordinates for products in a combinatorial library based on features of corresponding building blocks, the method comprising the steps of:

(1) obtaining mapping coordinates for a subset of products in the combinatorial library, wherein distances between the mapping coordinates represent relationships between the products;

(2) obtaining building block features for the subset of products in the combinatorial library;

(3) using a supervised machine learning approach to infer a mapping function *f* that transforms the building block features for each product in the subset of products to a corresponding mapping coordinate for each building block feature of each product in the subset of products; and

(4) encoding the mapping function *f* in a computer readable medium, whereby the mapping function *f* is used to generate coordinates corresponding to additional products in the combinatorial library from building block features associated with the additional products.

2. (Original) The method according to claim 1, further comprising the step of:

(5) providing building block features for at least one additional product to the mapping function *f* wherein the mapping function *f* outputs generated mapping coordinates for the additional product.

3. (Original) The method according to claim 1, wherein step (1) comprises generating the mapping coordinates for the subset of products.

4. (Currently Amended) The method according to claim 3, wherein step (1) further comprises the steps of:

(a) generating an initial set of mapping coordinates for the subset of products;

(b) selecting two products from the subset of products;

(c) determining a relationship between the two products;

(d) refining the initial set of mapping coordinates of one product selected in step (1)(b) based on the relationship and the corresponding distance between the products on the nonlinear map; and

(e) repeating steps (1)(b) and (1)(c) for additional products <u>until a stop criterion is obtained</u>.

5. (Original) The method according to claim 1, wherein step (1) comprises calculating the mapping coordinates for the subset of products using a dimensionality reduction algorithm.

6. (Original) The method according to claim 1, wherein step (1) comprises retrieving the mapping coordinates for the subset of products from a computer readable medium.

7. (Original) The method according to claim 1, wherein step (2) comprises the step of:

Using a laboratory measured value as a feature for each building block in at least one variation site in the combinatorial library.

8. (Original) The method according to claim 1, wherein step (2) comprises the step of:

using a computed value as a feature for each building block in at least one variation site in the combinatorial library.

9. (Original) The method according to claim 1, wherein at least some of the building block features represent reagents used to construct the combinatorial library.

10. (Previously presented) The method according to claim 1, wherein at least some of the building block features represent chemical fragments of reagents used to construct the combinatorial library.

11. (Previously presented) The method according to claim 1, wherein at least some of the building block features represent modified chemical fragments of reagents used to construct the combinatorial library.

12. (Original) The method according to claim 1, wherein the mapping function $f$ is encoded as a neural network.

13. (Previously presented) The method according to claim 1, wherein the mapping function $f$ is a set of mapping functions $f_1$ through $f_n$, each encoded as a neural network.

14. (Previously presented) A system for generating coordinates for products in a combinatorial library based on features of corresponding building blocks, comprising:

means for obtaining mapping coordinates for a subset of products in the combinatorial library, wherein distances between the mapping coordinates represent similarity/dissimilarity of the products;

means for obtaining building block features for the subset of products in the combinatorial library;

means for using a supervised machine learning approach to infer a mapping function *f* that transforms the building block features for each product in the subset of products to a corresponding mapping coordinate for each building block feature of each product in the subset of products; and

means for encoding the mapping function *f* in a computer readable medium, whereby the mapping function *f* is used to generate coordinates corresponding to additional products in the combinatorial library from building block features associated with the additional products.

15. (Original) The system of claim 14, further comprising:

means for providing building blocks features for at least one additional product to the mapping function *f*, wherein the mapping function *f* outputs generated mapping coordinates for the additional product.

16. (Currently Amended) The system of claim 14, wherein said means for obtaining mapping coordinates comprises:

means for generating an initial set of mapping coordinates for the subset of products;

means for selecting two products from the subset of products;

means for determining a relationship between the two products;

means for refining the initial set of mapping coordinates of one product selected based on the relationship and the corresponding distance between the products on the nonlinear map; and

means for continuously selecting two products at a time and refining the mapping coordinates of at least one product selected until a stop criterion is obtained.

17. (Original) The system of claim 14, wherein a laboratory measured value is used as a feature for each building block in at least one variation site in the combinatorial library.

18. (Original) The system of claim 14, wherein a computed value is used as a feature for each building block in at least one variation site in the combinatorial library.

19. (Original) The system of claim 14, wherein at least some of the building block features represent reagents used to construct the combinatorial library.

20. (Previously presented) The system of claim 14, wherein at least some of the building block features represent chemical fragments of reagents used to construct the combinatorial library.

21. (Previously presented) The system of claim 14, wherein at least some of the building block features represent modified chemical fragments of reagents used to construct the combinatorial library.

22. (Original) The system of claim 14, wherein the mapping function $f$ is encoded as a neural network.

23. (Previously presented) The system of claim 14, wherein the mapping function $f$ is a set of mapping functions $f_1$ through $f_n$ each encoded as a neural network.

24. (Currently Amended) A computer program product for generating coordinates for products in a combinatorial library based on features of corresponding building blocks, said computer program product comprising a computer useable medium having computer program logic recorded thereon for controlling a processor, said computer program logic comprising:

a procedure that enables said processor to obtain mapping coordinates for a subset of products in the combinatorial library, wherein distances between the mapping coordinates represent similarity/dissimilarity of the products;

a procedure that enables said processor to obtain building block features for the subset of products in the combinatorial library;

a procedure that enables said processor to use a supervised machine learning approach to infer a mapping function *f* that transforms the building block features for each product in the subset of products to a corresponding mapping coordinate for each building block feature of each product in the subset of products; and

a procedure that enables said processor to encode the mapping function *f* in a computer readable medium, whereby the mapping function *f* is used to generate coordinates corresponding to additional products in the combinatorial library from building block features associated with the additional products.

25. (Original) The computer program product of claim 24, further comprising:

a procedure that enable said processor to provide building blocks features for at least one additional product to the mapping function *f*, wherein the mapping function *f* outputs generated mapping coordinates for the additional product.

26. (Currently Amended) The computer program product of claim 24, wherein said procedure that enables said processor to obtain mapping coordinates comprises:

a procedure that enables said processor to generate an initial set of mapping coordinates for the subset of products;

a procedure that enables said processor to select two products from the subset of products;

a procedure that enables said processor to determine a relationship between the two products;

a procedure that enable said processor to refine the initial set of mapping coordinates of at least one product selected based on the relationship and the corresponding distance between the products on the nonlinear map; and

a procedure that enables said processor to continue selecting two products at a time and refining the mapping coordinates of at least one product selected until a stop criterion is obtained.

27. (Original) The computer program product of claim 24, wherein a laboratory measure value is used as a feature for each building block in at least one variation site in the combinatorial library.

28. (Original) The computer program product of claim 24, wherein a computed value is used as a feature for each building block in at least one variation site in the combinatorial library.

29. (Original) The computer program product of claim 24, wherein at least some of the building block features represent reagents used to construct the combinatorial library.

30. (Previously presented) The computer program product of claim 24, wherein at least some of the building block features represent chemical fragments of reagents used to construct the combinatorial library.

31. (Previously presented) The computer program product of claim 24, wherein at least some of the building block features represent modified chemical fragments of reagents used to construct the combinatorial library.

32. (Original) The computer program product of claim 24, wherein the mapping function $f$ is encoded as a neural network.

33. (Previously presented) The computer program product of claim 24, wherein the mapping function $f$ is a set of mapping functions $f_1$ through $f_n$, each encoded as a neural network.

34. (Cancelled)

35. (Cancelled)

36. (Currently Amended) The method of claim 1, wherein step (3) comprises:

(a) placing the selected training subset of products on an $m$-dimensional nonlinear map using randomly assigned coordinates;

(b) selecting a pair of the products having a similarity relationship;

(c) revising the coordinates of at least one of the selected pair of products based on the similarity relationship and the corresponding distance between the products on the nonlinear map; and

(d) repeating steps (b) and (c) for additional pairs of the products until the distances between the products on the $m$ dimensional nonlinear map are representative of the similarity relationships between the products.

37. (Cancelled)

38. (New) A method for generating coordinates for products in a combinatorial library based on features of corresponding building blocks, the method comprising the steps of:

(1) obtaining mapping coordinates for a subset of products in the combinatorial library, wherein distances between the mapping coordinates represent similarity/dissimilarity relationships between the products;

(2) obtaining building block features for the subset of products in the combinatorial library;

(3) using a supervised machine learning approach to infer a mapping function *f* that transforms the building block features for each product in the subset of products to a corresponding mapping coordinate for each building block feature of each product in the subset of products; and

(4) encoding the mapping function *f* in a computer readable medium, whereby the mapping function *f* is used to generate coordinates corresponding to additional products in the combinatorial library from building block features associated with the additional products.